Stat 992: Lecture 21
Diffusion smoothing on sphere.

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Problem 16. What is the heat kernel on a unit sphere ?
Solution. Read S. Rosenberg's The Laplacian on a Riemannian Manifold (1997 Cambridge University Press), I Chavel's Eigenvalues in Riemannian geometry (Academic Press, 1984), E.B. Davies' Heat kernels and spectral theory (Cambridge University Press, 1989). P. Olver and C. Shakiban's Fundamentals of Applied Mathematics, Prentice-Hall, in preparation.

1. *Diffusion on sphere.* Following lecture 7 and 20, we show the construction of heat kernel on a unit sphere. We have already showed how to construct it in implicit numerical scheme using the iterated kernel smoothing on manifolds. We may use spherical coordinate system:

$$x = \sin\theta\cos\psi,\ y = \sin\theta\sin\psi,\ z = \cos\theta.$$

On a unit sphere $p = (x, y, z) \in S^2$, heat kernel K_t must satisfy isotropic heat equation

$$\frac{\partial K_t}{\partial t} = \Delta_{S^2} K_t.$$

where

$$\Delta_{S^2} = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial^2\psi}.$$

It should satisfy the following three conditions $K_t(p, q) = K_t(q, p)$, $\lim_{t\to 0} K_t(p, q) = \delta(p - q)$ and $K_t(p, q) = \int_M K_s(p, r)K_{t-s}(r, q)\ dr$. Then the following PDE

$$\frac{\partial f}{\partial t} = \Delta_{S^2} f$$

with initial condition $f(0, p) = Y(p)$ has a unique solution

$$f(t, p) = \int_{S^2} K_t(p, q)Y(p)\ d\mu(p).$$

In lecture 20, we showed how to solve it numerically.

2. *Spherical Helmholtz equation.* We will follow lecture 11. In the previous lecture, we showed the metric to be $g_{11} = 1, g_{12} = g_{21} = 0, g_{22} = \sin^2\theta$. Define $L^2(S^2, g)$ with respect to the Riemannian metric g with inner product

$$\langle f, g\rangle = \int_{S^2} f(p)g(p)\ d\mu(p).$$

where the Lebesgue measure on a sphere is given by

$$d\mu = \sqrt{\det g}\ d\theta d\psi = \sin\theta d\theta d\psi.$$

This is the area element you must have seen it in vector calculus course. Note that $\int_{S^2}\ d\mu = 4\pi$, the area of the unit sphere.

The gradient $\nabla : C^\infty(S^2) \to T_p(S^2)$ in local coordinates is given by

$$\begin{aligned}\nabla f &= \sum_{i,j} g^{ij}\frac{\partial f}{\partial u^j}\frac{\partial p}{\partial u^i}\\ &= \frac{\partial f}{\partial\theta}\frac{\partial p}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial f}{\partial\psi}\frac{\partial p}{\partial\psi}.\end{aligned}$$

Then it can be shown that

$$\langle\Delta_{S^2} f, g\rangle = -\langle\nabla f, \nabla g\rangle = \langle f, \Delta_{S^2} g\rangle$$

So the spherical Laplacian is compact self-adjoint operator and it should have eigenvalues λ_j and eigenfunctions H_j such that

$$\Delta_{S^2} H_j(p) = \lambda_j H_j(p)$$

and $0 = |\lambda_0| \le |\lambda_1| \le |\lambda_2| \cdots$. To solve for eigenvalues and eigenfunctions of Laplacian, we need to solve the *spherical Helmholtz equation* given by

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\Big(\sin\theta\frac{\partial H}{\partial\theta}\Big) + \frac{1}{\sin^2\theta}\frac{\partial^2 H}{\partial^2\psi} - \lambda H = 0$$

Let us use the separation of variable technique: $H(\theta, \psi) = \alpha(\theta)\beta(\psi)$. Then substituting the term, we get

$$\sin^2\theta\frac{\alpha''}{\alpha} + \cos\theta\sin\theta\frac{\alpha'}{\alpha} - \sin^2\theta\lambda = -\frac{\beta''}{\beta} = c$$

Note that the left side is a function of θ while the right side is a function of ψ. The only way both side equal is when they are constant c.

The right hand side is trivial to solve:

$$\beta'' + c\beta = 0$$

Since $\beta(\psi)$ must be a periodic function with period 2π, the solutions are

$$\beta(\psi) = \cos(m\psi),\ \sin(m\psi)$$

where $m = \sqrt{c} = 0, 1, 2, \cdots$.

The left hand side is not so obvious to solve. We will change variable $t = \cos\theta$ and let

$$\alpha(\theta) = \alpha(cos^{-1} t) = P(t).$$

From the chain rule,

$$\alpha' = -\sqrt{1-t^2}P',$$

$$\alpha'' = (1-t^2)P'' - tP'.$$

Substituting these into the left side, we get

$$(1-t^2)^2P'' - 2t(1-t^2)P' - [\lambda(1-t^2) + m^2]P = 0$$

which is the *Legendre equation*. This is a well known ordinary differential equation (ODE) and its solution is the *Legendre functions*. Note that the solution is defined in the domain $-1 \leq t = \cos\theta \leq 1$ and we give boundary condition $|P(-1)| < \infty, |P(1)| < \infty$. For $m = 0$, $P_n(t) = \frac{1}{2^n n!}\frac{d^n}{dt^n}(t^2 - 1)^n, n = 0, 1, 2, \cdots$ are the Legendre polynomials. For general $m > 0$, the Legendre functions are constructed in the following way

$$P_n^m(t) = (1-t^2)^{m/2}\frac{d^m}{dt^m}P_n(t),\ n = m, m+1, \cdots$$

Even ordered Legendre functions are polynomials but for odd ordered functions there is an additional factor $\sqrt{1-t^2}$. In summarizing the result, the complete set of solutions for the left hand side is

$$\alpha(\theta) = P_n^m(\cos\theta), n = m, m+1, \cdots.$$

For instance $P_0^0 = 1, P_1^0 = \cos\theta, P_1^1 = -\sin\theta, P_2^0 = \frac{1}{4} + \frac{3}{4}\cos 2\theta, \cdots$.

3. *Spherical harmonics.* By combining the solution from both ODEs, we have the complete set of solution to the spherical Helmholtz equation gives spherical harmonics:

$$H_n^m(\theta, \psi) = \cos(m\psi)P_n^m(\cos\theta),$$

$$\widetilde{H}_n^m(\theta, \psi) = \sin(m\psi)P_n^m(\cos\theta)$$

where $n = 0, 1, 2, \cdots, m = 0, 1, \cdots, n$. The spherical harmonics satisfy

$$\Delta_{S^2}H_n^m + n(n+1)Y_n^m = \Delta_{S^2}\widetilde{H}_n^m + n(n+1)Y_n^m = 0.$$

Note that $\widetilde{H}_n^0 = 0$. The corresponding eigenvalues are $\lambda_n = -n(n+1)$. These harmonics are orthogonal but not normalized. It can be shown that

$$\|H_n^0\|^2 = \frac{4\pi}{2n+1}, \|H_n^m\|^2 = \|\widetilde{H}_n^m\|^2 = \frac{2\pi(n+m)!}{(2n+1)(n-m)!}.$$

We will assume H_n^m and $\widetilde{H}_n^m$ are normalize by dividing by the norms. Then the spherical harmonics can span any function $f \in L^2(S^2)$ so that

$$f(\theta, \psi) = \sum_{n=0}^{\infty}\sum_{m=0}^{n} c_{m,n}\big[H_n^m + \widetilde{c}_{m,n}\widetilde{H}_n^m\big]$$

where $c_{m,n} = \langle f, H_n^m\rangle$, $\widetilde{c}_{m,n} = \langle f, \widetilde{H}_n^m\rangle$. For simplicity let us order spherical harmonics H_n^m and $\widetilde{H}_n^m$ by H_j. Then it can be shown that the spherical heat kernel can be extended as

$$K_t(p, q) = \sum_{j=0}^{\infty} e^{-\lambda_j t}H_j(p)H_j(q).$$

Hence solution to diffusion smoothing on the unit sphere is exactly expressed as

$$f(t, q) = \sum_{j=0}^{\infty} e^{-\lambda_j t}H_j(q)\int_0^{2\pi}\int_0^{\pi} H_j(p)Y(p)\sin\theta\ d\theta d\psi.$$

Problem 32. Simplify the above expression. Please make sure your simplified expression and the above derivation is correct by directly showing it satisfies the heat equation.

Problem 33. Following above derivation, solve heat equation on a unit circle S^1. Show every detail.